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# Monte Carlo Calculation of the Thermodynamic Properties of a One-Dimensional Fermion Lattice Model

Hans De Raedt and Ad Lagendijk<sup>1,2</sup>

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The generalized Trotter formula is used to derive two different classical representations of the partition function of a one-dimensional fermion model. Short-chain calculations are used to study the corresponding approximants for the energy and specific heat. A Monte Carlo technique has been used to calculate the temperature-dependent properties of a chain of 64 sites.

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**KEY WORDS:** Monte Carlo; fermion model; trotter formula; one-dimensional; partition function; classical representation.

## 1. INTRODUCTION

Recently Suzuki<sup>(1)</sup> demonstrated that the generalized Trotter formula<sup>(2,3)</sup> can be used to map the partition function of a  $d$ -dimensional quantum spin-1/2 model onto the partition function of a  $(d + 1)$ -dimensional Ising model with four-spin interactions, and similar mappings have been derived for fermion models and more complicated spin systems.<sup>(4)</sup> This approach to quantum statistical mechanics is very appealing because, in principle, it is possible to calculate the temperature-dependent properties without diagonalizing the full Hamiltonian.<sup>(5)</sup> In practice, the relevant quantities of the quantum system might be obtained by a Monte Carlo simulation of the classical model.<sup>(5)</sup> Because there is no unique classical representation for a given quantum Hamiltonian, it is necessary to study the convergence properties of different representations by means of exact calculations for

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small systems before one adds the complication of the Monte Carlo procedure.

In this paper we carry out such a program for the one-dimensional spinless fermion lattice model described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \quad (1.1a)$$

$$\mathcal{H}_0 = -t \sum_{l=1}^M c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l, \quad c_l = c_{l+M}, \quad t > 0 \quad (1.1b)$$

$$\mathcal{H}_1 = v \sum_{l=1}^M c_l^\dagger c_l c_{l+1}^\dagger c_{l+1} = v \sum_{l=1}^M n_l n_{l+1} \quad (1.1c)$$

The operator  $c_l^\dagger$  creates a fermion at site  $l$  and  $n_l$  denotes the number operator at site  $l$ . The energy associated with the hopping motion of the particles is given by  $\mathcal{H}_0$  and the interaction between nearest neighbors is determined by  $\mathcal{H}_1$ . It is well known that Hamiltonian (1.1) is equivalent to the spin-1/2 Ising-Heisenberg chain if  $M \rightarrow \infty$ .<sup>(6)</sup> The model is also a familiar starting point in the description of some phenomena observed in charge-transfer salts.<sup>(7,8)</sup>

In order to calculate the partition function of model (1.1) we use the Trotter formula<sup>(2,3)</sup> for the bounded operators  $A_k$ ,

$$\exp\left(\sum_{k=0}^n A_k\right) = \lim_{m \rightarrow \infty} \left[ \exp\left(\frac{A_0}{m}\right) \cdots \exp\left(\frac{A_n}{m}\right) \right]^m \quad (1.2)$$

for two different decompositions of Hamiltonian (1.1). The basic idea of using (1.2) is to calculate temperature-dependent quantities for given  $m$  and to study the convergence of the results as  $m$  increases. It is the purpose of this work to show that this new computational technique can be very useful for the numerical determination of thermodynamic properties of quantum systems.

In Sections 2 and 3, we derive the relevant formula for the energy, specific heat, and density-density correlation functions using two different classical representations. Exact calculations for short chains for several values of  $m$  will be presented in Section 4, and the results will be compared with the solution obtained by diagonalizing the full Hamiltonian. In Section 5, we show how the standard Monte Carlo method should be modified in order to be applicable to the quantum case and we present results for long chains ( $M = 64$ ). The conclusions of our work are summarized in Section 6.

## 2. FIRST FORMULATION

Taking  $n = 1$ ,  $A_0 = -\beta \mathcal{H}_0$ , and  $A_1 = -\beta \mathcal{H}_1$  in Eq. (1.2) we have

$$Z \equiv \lim_{m \rightarrow \infty} Z_m^{(1)} \quad (2.1a)$$

$$Z_m^{(1)} = \text{Tr}(e^{-\beta \mathcal{H}_0/m} e^{-\beta \mathcal{H}_1/m})^m \quad (2.1b)$$

$$\begin{aligned} &= \sum_{\{\phi\}} \langle \phi_1 | e^{-\beta \mathcal{H}_0/m} | \phi_2 \rangle \langle \phi_2 | e^{-\beta \mathcal{H}_1/m} | \phi_2 \rangle \\ &\times \cdots \langle \phi_m | e^{-\beta \mathcal{H}_0/m} | \phi_1 \rangle \langle \phi_1 | e^{-\beta \mathcal{H}_1/m} | \phi_1 \rangle \end{aligned} \quad (2.1c)$$

where  $\phi_i \equiv \phi_i(x_{1,i} \cdots x_{N,i}) = c_{x_{1,i}}^+ \cdots c_{x_{N,i}}^+ |0\rangle$ ,  $N$  being the number of particles. We have used the fact that  $\phi_i$  is an eigenfunction of  $\mathcal{H}_1$ . As  $\mathcal{H}_0$  can be diagonalized by Fourier transformation, the matrix elements  $\langle \phi_i | \exp(-\beta \cdot \mathcal{H}_0/m) | \phi_{i+1} \rangle$  can be evaluated explicitly, and we obtain

$$Z_m^{(1)} = \sum_{\{P_j\}} \sum_{\{x_{l,j}\}} \rho(\{x_{l,j}\}, \{P_j\}) \text{sign}(P_1 \cdots P_j) \quad (2.2a)$$

$$\rho(\{x_{l,j}\}, \{P_j\}) = \prod_{j=1}^m \prod_{l=1}^N J(2t\beta^*, y_{l,j}) \exp \left[ -v\beta^* \sum_{l'} \delta_{(x_{l,j} - x_{l',j}) \bmod M, l} \right] \quad (2.2b)$$

where

$$J(\alpha, x) = \frac{1}{M} \sum_{k=1}^M \cos \frac{2\pi kx}{M} \exp \left( \alpha \cos \frac{2\pi k}{M} \right) \quad (2.2c)$$

and

$$y_{l,j} = x_{l,j} - x_{P_{j+1}l,j+1} \quad (2.2d)$$

The position of the  $(l, j)$ th particle on the two-dimensional lattice has been denoted by  $x_{l,j} = x_{l+Mj} = x_{l,j+m}$ ,  $\beta^* = \beta/m$  and  $P_j$  is a permutation operator acting on the set  $\{1, \dots, N\}$ .

In Eq. (2.2) the sum over  $\{x_{l,j}\}$  has to be taken such that there is at most one particle at a given site. By a change of summation variables, Eq. (2.2) can be written as

$$Z_m^{(1)} = \sum_P \sum_{\{x_{l,j}\}} \rho(\{x_{l,j}\}, P) \text{sign}(P) \quad (2.3a)$$

$$\begin{aligned} \rho(\{x_{l,j}\}, P) &= \prod_{j=1}^m \prod_{l=1}^N J(2t\beta^*, x_{l,j} - x_{l,j+1}) \\ &\times \exp \left[ -v\beta^* \sum_{l'} \delta_{(x_{l,j} - x_{l',j}) \bmod M, l} \right] \end{aligned} \quad (2.3b)$$

where in this case  $x_{l,m+1} = x_{Pl,1}$ . Thus we have shown that  $Z_m^{(1)}$  is a genuine discrete version of Feynman's path-integral representation for the partition function of a fermion model.<sup>(9)</sup> We have found Eq. (2.2) to be more convenient for numerical applications because permutation operators appear in a more symmetric manner.

The energy can be obtained from

$$E_m^{(1)} = - \frac{\partial}{\partial \beta} \ln Z_m^{(1)} \quad (2.4a)$$

$$= - \frac{1}{Z_m^{(1)}} \sum_{\{P_j\}} \sum_{\{x_{lj}\}} \rho(\{x_{lj}\}, \{P_j\}) \text{sign}(P_1 \cdots P_m) e_m(\beta) \quad (2.4b)$$

$$e_m(\beta) = \sum_{j=1}^m \sum_{l=1}^N \left[ \frac{t}{m} \frac{J(2t\beta^*, y_{lj} - 1) + J(2t\beta^*, y_{lj} + 1)}{J(2t\beta^*, y_{lj})} - \frac{v}{m} \sum_{l'} \delta_{(x_{lj} - x_{l',j}) \bmod M, 1} \right] \quad (2.4c)$$

The specific heat is given by

$$C_m^{(1)} = -\beta^2 \frac{\partial}{\partial \beta} E_m^{(1)} \quad (2.5a)$$

$$= \beta^2 \left[ \frac{1}{Z_m^{(1)}} \sum_{\{P_j\}} \sum_{\{x_{lj}\}} \rho(\{x_{lj}\}, \{P_j\}) \text{sign}(P_1 \cdots P_m) \times [\{e_m(\beta)\}^2 + e'_m(\beta)] - \{E_m^{(1)}\}^2 \right] \quad (2.5b)$$

where

$$e'_m(\beta) = \left( \frac{t}{m} \right)^2 \left\{ 2mN + \sum_{j=1}^m \sum_{l=1}^N \frac{J(2t\beta^*, y_{lj} - 2) + J(2t\beta^*, y_{lj} + 2)}{J(2t\beta^*, y_{lj})} - \left[ \frac{J(2t\beta^*, y_{lj} - 1) + J(2t\beta^*, y_{lj} + 1)}{J(2t\beta^*, y_{lj})} \right]^2 \right\} \quad (2.5c)$$

Another interesting quantity to sample is the static structure factor  $S(q)$  which is the Fourier transform of the density-density correlation function,

$$\langle n_i n_{i+k} \rangle = \frac{1}{mM} \sum_{\{P_j\}} \sum_{\{x_{lj}\}} \rho(\{x_{lj}\}, \{P_j\}) \text{sign}(P_1 \cdots P_m) \times \sum_{j=1}^m \sum_{l=1}^M \sum_{l'=1}^M \delta_{|x_{lj} - x_{l',j}| \bmod M, k} \quad (2.6)$$

We close this section with some general remarks. An important feature of this formulation is that<sup>(9)</sup>

$$Z_{2^p}^{(1)} \geq Z_{2^{p+1}}^{(1)} \geq Z \quad (2.7)$$

which implies that we obtain exact lower bounds for the free energy for certain choices of  $m$ . It is trivial to verify that  $Z_m^{(1)} = Z$  if  $t \cdot v = 0$ . Because we have used a representation for which  $\mathcal{H}_1$  is diagonal, it is easy to include more-distant interactions in this formulation. It is also straightforward to derive expressions for a two- or three-dimensional lattice.

### 3. SECOND FORMULATION

Here we take in Eq. (1.2)  $n = M$  and

$$A_k = \beta t (c_k^+ c_{k+1} + c_{k+1}^+ c_k) - \beta v n_k n_{k+1} \quad (3.1)$$

The two-fermion Hamiltonian (3.1) can be diagonalized, and because of the local character of the decomposition, the approximant  $Z_m^{(2)}$  takes the form

$$Z_m^{(2)} = \sum_{\{n_{lj}\}} \tilde{\rho}(\{n_{lj}\}) \quad (3.2a)$$

$$\begin{aligned} \tilde{\rho}(\{n_{lj}\}) &= \prod_{j=1}^{2m+1} \prod_{l=1}^{M-1} T(n_{lj+1}, n_{l+1,j}; n_{lj+2}, n_{l+1,j+1}) \\ &\times (1 - 2|n_{M,j} - n_{M,j+1}|)^{N-1} \end{aligned} \quad (3.2b)$$

where  $n_{lj} = n_{l+M,j} = n_{l,j+2m+1} = 1$  if the site  $(l, j)$  of the two-dimensional lattice is occupied, otherwise  $n_{lj} = n_{l+M,j} = n_{l,j+2m+1} = 0$ . The second factor in the product (3.2b) would not be present if we had not chosen periodic boundary conditions. If we put  $\alpha = 2n_1 + n_2 + 1$  and  $\beta = 2n'_1 + n'_2 + 1$  we can write  $T$  in a matrix notation

$$T(n_1, n_2; n'_1, n'_2) \equiv T_{\alpha\beta} \quad (3.3a)$$

$$[T_{\alpha\beta}] = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cosh(t\beta^*) & \sinh(t\beta^*) & 0 \\ 0 & \sinh(t\beta^*) & \cosh(t\beta^*) & 0 \\ 0 & 0 & 0 & e^{-v\beta^*} \end{bmatrix} \quad (3.3b)$$

In the special case  $m = 1$ , it is possible to calculate the sum (3.2) analytically (see Appendix). We now proceed as in the previous section and obtain the following expressions for the energy, specific heat, and density-density

correlation functions:

$$E_m^{(2)} = - \frac{1}{Z_m^{(2)}} \sum_{\{n_{l,j}\}} \tilde{\rho}(\{n_{l,j}\}) \tilde{e}_m(\beta) \quad (3.4a)$$

$$\tilde{e}_m(\beta) = \sum_{l=1}^M \sum_{j=1}^{m+1} \frac{(\partial/\partial\beta) T(n_{l,j+1}, n_{l+1,j}; n_{l,j+2}, n_{l+1,j+1})}{T(n_{l,j+1}, n_{l+1,j}; n_{l,j+2}, n_{l+1,j+1})} \quad (3.4b)$$

$$C_m^{(2)} = \beta^2 \left[ \frac{1}{Z_m^{(2)}} \sum_{\{n_{l,j}\}} \tilde{\rho}(\{n_{l,j}\}) \left[ \{\tilde{e}_m(\beta)\}^2 + \frac{\partial}{\partial\beta} \tilde{e}_m(\beta) \right] - \{E_m^{(2)}\}^2 \right] \quad (3.4c)$$

$$\langle n_i n_{i+k} \rangle = \frac{1}{mM} \sum_{\{n_{l,j}\}} \tilde{\rho}(\{n_{l,j}\}) \left[ \sum_{j=1}^m \sum_{l=1}^M \sum_{l'=1}^M n_{l,j} n_{(l'+k) \bmod M, j} \right] \quad (3.4d)$$

Note that locality is an essential ingredient of this approach, and therefore it is difficult to include more-distant interactions in this formulation. A general feature of both formulations is that it is difficult to calculate quantities which cannot be expressed as a combination of derivatives of the partition function or which are not diagonal in the real-space basis.

Finally we want to mention that it is also possible to improve the approximation by decoupling the Hamiltonian in cells of three, four, or more sites. In the  $m = 1$  case, it is then possible to sum over all sites within each cell. This approach has some nice properties but it is outside the scope of this paper.

#### 4. SHORT CHAINS

For short chains ( $M \leq 8$ ) and small  $m$ , it is possible to sum over all possible configurations (and permutations) exactly. In general, this has to be done numerically but it is not difficult to calculate the relevant quantities to very high precision. In this section we discuss the convergence of the approximants, introduced in the previous sections, as a function of  $m$  and we compare the results with those obtained by diagonalizing the full Hamiltonian (1.1).

For all our numerical calculations we have taken  $t = 1$ ,  $v = 2$  and a half-filled band or  $N = M/2$ . For this particular choice of model parameters the ground-state of model (1) corresponds to the ground state of the antiferromagnetic spin-1/2 Heisenberg chain for which the exact ground-state energy for  $M \rightarrow \infty$  is known.<sup>(10)</sup> Furthermore the interaction  $\mathcal{H}_1$  and the free part  $\mathcal{H}_0$  are equally important, so that we are testing the method for the most difficult case.

**Table I. Exact Results for the Energy (Specific Heat) per Site for Two Particles and Four Sites Obtained from Eqs. (2.3)–(2.5). The Results for  $m = \infty$  are Obtained by Diagonalizing the Full Hamiltonian**

$m$	$\beta = 0.3$	$\beta = 0.5$	$\beta = 1$	$\beta = 2$
1	0.0447(0.0875)	– 0.1356(0.2017)	– 0.3941(0.2716)	– 0.4900(0.0863)
2	0.0531(0.0806)	– 0.1059(0.1698)	– 0.3149(0.2277)	– 0.4316(0.2599)
3	0.0547(0.0793)	– 0.0997(0.1622)	– 0.2900(0.1893)	– 0.3826(0.2359)
4	0.0553(0.0788)	– 0.0975(0.1595)	– 0.2802(0.1716)	– 0.3552(0.1775)
5	0.0555(0.0786)	– 0.0964(0.1582)	– 0.2754(0.1626)	– 0.3399(0.1336)
6	0.0557(0.0785)	– 0.0959(0.1574)	– 0.2728(0.1574)	– 0.3308(0.1040)
$\infty$	0.0560(0.0782)	– 0.0946(0.1558)	– 0.2666(0.1451)	– 0.3076(0.0187)

In Tables I and II we present some typical results for the first approach. For high temperatures (small  $\beta$ ), both the specific heat and the energy rapidly converge to the exact result ( $m \rightarrow \infty$ ). This could be expected because Eq. (2.1) becomes exact in the limit  $\beta/m \rightarrow 0$ . At very low temperatures ( $\beta = 2$ ) we still have reasonable convergence. One might argue that  $\beta = 2$  does not correspond to a very low temperature, but if we compare the ground-state energy of a chain of for example 4 sites ( $E_0 = -0.3090$ ) with the energy for  $\beta = 2$  ( $E = -0.3076$ ) it is clear that we are in the very low temperature regime indeed.

The corresponding results for the real-space decomposition are given in Tables III and IV. In general, the results converge slower to the exact values than in the other approach. At low temperatures the results for the specific heat do not converge at all for the values of  $m$  we could do in our calculation. We have found that the results for the correlation functions do not differ much, but the first approach does give slightly better results. For comparison, we have also included the exact ( $m = 1, M \rightarrow \infty$ ) results of the

**Table II. Exact Results for the Energy (Specific Heat) per Site for Four Particles and Eight Sites Obtained from Eqs. (2.3)–(2.5). The Results for  $m = \infty$  are Obtained by Diagonalizing the Full Hamiltonian**

$m$	$\beta = 0.3$	$\beta = 0.5$	$\beta = 1$	$\beta = 2$
1	0.1579(0.0856)	– 0.0286(0.2233)	– 0.3730(0.4679)	– 0.5765(0.2333)
2	0.1627(0.0815)	– 0.0091(0.1986)	– 0.2954(0.3679)	– 0.4796(0.3765)
3	0.1617(0.0806)	– 0.0051(0.1930)	– 0.2744(0.3283)	– 0.4272(0.2951)
$\infty$	0.1644(0.0800)	– 0.0017(0.1883)	– 0.2551(0.2865)	– 0.3595(0.0892)



**Table III. Exact Results for the Energy (Specific Heat) per Site for Two Particles and Four Sites Obtained from Eqs. (3.2)–(3.4). The Results for  $m = \infty$  are Obtained by Diagonalizing the Full Hamiltonian. The Rigorous  $m = 1, M \rightarrow \infty$  Results Can be Found in the Appendix**

$m$	$\beta = 0.3$	$\beta = 0.5$	$\beta = 1$	$\beta = 2$
1	0.0322(0.0992)	− 0.1942(0.2847)	− 0.6717(0.6830)	− 0.9615(0.3220)
2	0.0504(0.0830)	− 0.1163(0.1820)	− 0.3479(0.2613)	− 0.5775(1.4282)
3	0.0535(0.0803)	− 0.1039(0.1668)	− 0.2974(0.1737)	− 0.2852(− 0.8200)
4	0.0546(0.0793)	− 0.0998(0.1619)	− 0.2828(0.1566)	− 0.2718(− 0.6796)
5	0.0551(0.0789)	− 0.0979(0.1596)	− 0.2767(0.1512)	− 0.2814(− 0.4268)
6	0.0554(0.0787)	− 0.0969(0.1585)	− 0.2734(0.1489)	− 0.2889(− 0.2795)
$\infty$	0.0560(0.0782)	− 0.0946(0.1558)	− 0.2666(0.1451)	− 0.3076(0.0187)
$1(M \rightarrow \infty)$	0.2443(0.0846)	0.0493(0.2494)	− 0.4225(0.8215)	− 0.8958(0.7900)

Appendix in Tables III and IV. Thus, from a theoretical point of view, we would prefer to apply the Monte Carlo technique to the first formulation. It is amusing to point out that for the very short chains, for which the diagonalization of the Hamiltonian is possible, the results in our tables for the maximum values of  $m$  took about several million times more computer time than the exact-diagonalization results.

**5. MONTE CARLO CALCULATIONS**

If one wants to study the properties of long chains, it is not possible to diagonalize the full Hamiltonian or to perform an exact summation over all

**Table IV. Exact Results for the Energy (Specific Heat) per Site for Four Particles and Eight Sites Obtained from Eqs. (3.2)–(3.4). The Results for  $m = \infty$  are Obtained by Diagonalizing the Full Hamiltonian. The Rigorous  $m = 1, M \rightarrow \infty$  Results Can be Found in the Appendix**

$m$	$\beta = 0.3$	$\beta = 0.5$	$\beta = 1$	$\beta = 2$
1	0.1553(0.0904)	− 0.0544(0.2655)	− 0.5591(0.8647)	− 0.9565(0.3986)
2	0.1616(0.0826)	− 0.0155(0.2091)	− 0.3453(0.4937)	− 0.6762(0.9462)
3	0.1631(0.0812)	− 0.0079(0.1976)	− 0.2944(0.3715)	− 0.4678(0.2884)
$\infty$	0.1644(0.0800)	− 0.0017(0.1883)	− 0.2551(0.2865)	− 0.3595(0.0892)
$1(M \rightarrow \infty)$	0.2443(0.0846)	0.0493(0.2494)	− 0.4225(0.8215)	− 0.8958(0.7900)

possible configurations. Therefore, we will use a Monte Carlo technique to obtain the relevant quantities. At first sight, it seems very plausible that this can be done because there is the general statement that the partition function of a  $d$ -dimensional quantum model is equivalent to the partition function of a  $(d + 1)$ -dimensional classical model.<sup>(1)</sup> However, for practical applications, it is necessary that each contribution to the classical partition function is positive.<sup>(12)</sup> Otherwise, the transition probability for the Monte Carlo scheme would be negative. In general, this condition is only satisfied for a small class of models (such as ferromagnets). In this section, we slightly reformulate the original problem such that we can still apply the Monte Carlo method.

In the previous section, we have demonstrated that from a theoretical point of view, the first approach, in which the Hamiltonian is partitioned in kinetic and potential energy, is better than the second approach, in which the Hamiltonian is partitioned in real-space parts, and we now argue that the first formulation is also considerably simpler for practical applications. Examining matrix (3.3b) we see that a large number of its elements are zero<sup>3</sup> and consequently a large number of configurations do not contribute to the partition function (3.2). As it would be very inefficient to generate these configurations, an additional algorithm for finding nonzero configurations is required. In practice this means that one has to move several particles at the same time. Although several efficient algorithms can be derived, the main problem is that this algorithm should be used in each Monte Carlo step. In the first formulation, there are no zero contributions to the partition function, and therefore it is possible to move one particle at a time. This simplifies programming and decreases computation time considerably.

These considerations have led us to the conclusion that we should start from the “path-integral approach” for the actual simulation. We now present the essential steps of our calculation.<sup>(13)</sup> In order to have a positive transition probability we define the following average of a quantity  $A$ :

$$\ll A \gg = \text{Tr } \rho A / \text{Tr } \rho \quad (5.1)$$

where we used a shorthand notation for  $\rho = \rho(\{x_{lj}\}, \{P_j\})$  and  $\text{Tr}$  denotes the sum over all possible  $\{x_{lj}\}$  and  $\{P_j\}$ . As in Monte Carlo calculations of real classical models, the partition function itself is not of direct interest. The energy, specific heat, and correlation functions can be expressed

<sup>3</sup> We have chosen the model parameters such that each element of  $T$  is not negative. However, there are still negative contributions to  $Z_m^{(2)}$  because of periodic boundary conditions.

entirely in terms of the averages defined in Eq. (5.1):

$$E_m^{(1)} = \ll \text{sign}(P_1 \cdots P_m) e_m(\beta) \gg / \ll \text{sign}(P_1 \cdots P_m) \gg \quad (5.2a)$$

$$C_m^{(1)} = \beta^2 \left[ \ll \text{sign}(P_1 \cdots P_m) [\{e_m(\beta)\}^2 + e'_m(\beta)] \gg \right. \\ \left. \times \{ \ll \text{sign}(P_1 \cdots P_m) \gg \}^{-1} - \{E_m^{(1)}\}^2 \right] \quad (5.2b)$$

$$\langle n_i n_{i+k} \rangle = \frac{1}{mM} \sum_{j=1}^m \sum_{l=1}^N \sum_{l'=1}^N \ll \text{sign}(P_1 \cdots P_m) \delta_{(x_{lj} - x_{l'j}) \bmod M, k} \gg \\ \times \ll \text{sign}(P_1 \cdots P_m) \gg^{-1} \quad (5.2c)$$

Because  $\rho$  is positive [see Eqs. (2.2b) and (2.2c)], we only have to generate a Markov chain of configurations such that the transition probability,  $p$ , is given by  $p = \rho(\text{new configuration}) / \rho(\text{old configuration})$ .<sup>(12)</sup> Thus we still use the standard Monte Carlo method to calculate the averages as defined in Eq. (5.1) and we then use Eqs. (5.2) to obtain the thermodynamic properties of the fermion model. It is interesting to note that  $\text{Tr} \rho$  is the partition function of a boson model with a hard-core interaction that prevents two or more particles from occupying the same site.

The Markov chain is generated as follows. Select a particle  $(l, j)$  randomly and move it one position to the left (right) with probability  $1/2$ . If the new position is already occupied by another particle, move that particle one position to the right (left), and modify the corresponding permutations accordingly. Calculate the transition probability  $p$  and accept the new configuration if  $p \geq r$  ( $0 \leq r \leq 1$ ,  $r$  being a random number). Instead of moving a particle, one might also change a permutation (chosen at random) and then calculate the transition probability. This has been built in in our program, but we have found that this has a negligible effect on the results.

We now discuss the results of a simulation of a system of 32 particles on 64 sites. In each run, 2000 samples were taken and the first 4,000,000 Monte Carlo steps were discarded by the sampling procedure. For each temperature we took the average of the results of three independent runs. Instead of varying  $m$  for each temperature, we have taken  $m$  such that  $m/\beta = 16$  (except for  $\beta = 2$ , where we also have taken  $m = 36$ ), because we know from our previous calculation<sup>(13)</sup> for a chain of 32 sites that for this choice of  $m$  the convergence to the exact values is already very good. In Table V, we present the data for the energy and specific heat per site for the fermion model (denoted by  $E_F$  and  $C_F$ ) and for the associated boson

**Table V. Monte Carlo Results for the Energy and Specific Heat of the Fermion Model ( $E_F, C_F$ ) and the Associated Boson Model ( $E_B, C_B$ ) for a System of 32 Particles and 64 Sites**

	$\beta = 0.5$	$\beta = 1$	$\beta = 1.5$	$\beta = 2$	$\beta = 2(m = 36)$
$E_F$	$0.075 \pm 0.008$	$-0.192 \pm 0.009$	$-0.293 \pm 0.002$	$-0.348 \pm 0.011$	$-0.345 \pm 0.010$
$E_B$	$0.035 \pm 0.008$	$-0.230 \pm 0.007$	$-0.332 \pm 0.004$	$-0.387 \pm 0.008$	$-0.385 \pm 0.007$
$C_F$	$0.189 \pm 0.003$	$0.32 \pm 0.05$	$0.33 \pm 0.1$	$-0.1 \pm 0.2$	$0.04 \pm 0.19$
$C_B$	$0.202 \pm 0.003$	$0.37 \pm 0.01$	$0.40 \pm 0.05$	$0.21 \pm 0.08$	$0.27 \pm 0.08$

model (denoted by  $E_B$  and  $C_B$ ). Except for  $C_F$  at  $\beta \geq 1.5$ , the statistical errors are rather small. Comparing the exact ground-state energy  $E_0 = -0.386$  with  $E_F(\beta = 2) = -0.345 \pm 0.010$  we conclude that  $\beta = 2$  corresponds to a very low temperature indeed. In this temperature region, the specific heat  $C_F$  is very small and difficult to sample. In Fig. 1 we have plotted the Fourier transformed density-density correlation function

$$S(q) = \sum_{k=1}^M \cos(kq) \langle n_i n_{i+k} \rangle - \delta_{q,0} N^2 / M, \quad q = 0, \frac{2\pi}{M}, \dots, \frac{2\pi(M-1)}{M} \quad (5.3)$$

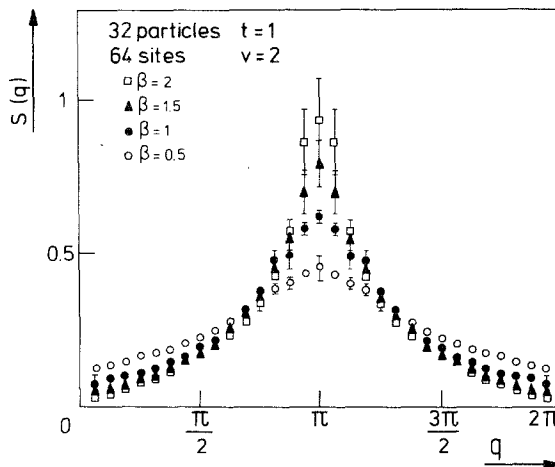


Fig. 1. Monte Carlo results for the Fourier-transformed density-density correlation function of the fermion model. The number of particles is 32, the number of sites is 64. If no error bars are shown, the statistical errors are too small to be drawn on this scale.

for different temperatures. If we compare these data with those of a system of 16 particles on 32 sites, we find very good agreement and therefore we believe it is not meaningful to study longer chains. As in Ref. 13 we observe that the statistical errors are larger for lower temperatures and that the maximum of  $S(q)$  varies slowly as a function of temperature. This is quite different for the (classical)  $t = 0$  model, because in this model without hopping,  $S(q)$  changes by a factor of about 2 if  $\beta$  goes from 1 to 2. Apparently, the correlation functions clearly demonstrate the effect of quantum fluctuations. We also want to stress<sup>(13)</sup> the fact that the Hartree–Fock approximation yields qualitatively incorrect results for the correlation functions of this strongly interacting many-body system.

## 6. CONCLUSIONS

We have calculated the temperature-dependent properties of a strongly interacting one-dimensional fermion lattice model. Starting from the generalized Trotter formula, we derived two essentially different classical representations for the partition function. For short chains, exact summations have been performed to compare the two different approximants with results obtained by diagonalizing the full Hamiltonian. The best approximant, which turned out to be the equivalent of Feynman's path-integral representation for the partition function, has been found to be most suited for numerical applications.

A Monte Carlo scheme has been devised to simulate the fermion model on a computer, and results for the energy and specific heat per site and the density–density correlation function have been presented. Quantum effects and the strong interactions are found to have an important effect on the behavior of the correlation functions.

In our opinion, the approach followed in the present paper can be used to study other quantum models, such as the extended Hubbard model and the antiferromagnetic spin-1/2 Heisenberg chain, as well.

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## APPENDIX

For analytic calculations, it is convenient to replace  $A_k$  of Eq. (3.1) by  $A_k - \beta\mu(n_k + n_{k+1})/2$ . Here,  $\mu$  denotes the chemical potential. The matrix

$T$  now takes the form

$$[T_{\alpha\beta}] = e^{\beta^* \mu/2} \begin{bmatrix} e^{-\beta^* \mu/2} & 0 & 0 & 0 \\ 0 & \cosh(\beta^* t) & \sinh(\beta^* t) & 0 \\ 0 & \sinh(\beta^* t) & \cosh(\beta^* t) & 0 \\ 0 & 0 & 0 & e^{\beta^* (\mu/2 - v)} \end{bmatrix} \quad (\text{A.1})$$

A large number of configurations do not contribute to the partition function  $Z_m^{(2)}$  because of the relatively large number of zero elements in  $T_{\alpha\beta}$ . The special case  $m = 1$  ( $\beta = \beta^*$ ) can be treated analytically by observing that  $T(n_1, n_2; n'_1, n'_2) \neq 0$  if, and only if,  $n_1 = n'_1$  and  $n_2 = n'_2$  or  $n_1 \neq n'_1$  and  $n_2 \neq n'_2$ . Then,  $Z_1^{(2)}$  can be written as

$$Z_1^{(2)} = e^{\beta \mu M/2} \sum_{\{n_i\}} T_1(n_1, n_2) T_1(n_2, n_3) \cdots T_1(n_{M-1}, n_M) T_1(n_M, n_1) \\ + e^{\beta \mu M/2} \sum_{\{n_i\}} T_2(n_1, n_2) T_2(n_2, n_3) \cdots T_2(n_{M-1}, n_M) T_2(n_M, n_1) \quad (\text{A.2a})$$

where

$$T_1(n_1, n_2) = \begin{bmatrix} e^{-\beta \mu/2} & \cosh(\beta t) \\ \cosh(\beta t) & e^{\beta(\mu/2 - v)} \end{bmatrix} \quad (\text{A.2b})$$

and

$$T_2(n_1, n_2) = \begin{bmatrix} \sinh(\beta t) & 0 \\ 0 & \sinh(\beta t) \end{bmatrix} \quad (\text{A.2c})$$

Here we have used the same convention as in Eq. (3.4). The sum (A.2a) can be evaluated by means of the transfer-matrix technique and the result reads

$$Z_1^{(2)} = \lambda_1^M + \lambda_2^M + 2 \{ e^{\beta \mu/2} \sinh(\beta t) \}^M \quad (\text{A.3a})$$

where

$$\lambda_{1,2} = \frac{1}{2} \left\{ 1 + e^{\beta(\mu - v)} \pm \left[ (1 - e^{\beta(\mu - v)})^2 + 4e^{\beta \mu} \cosh^2 \beta t \right]^{1/2} \right\} \quad (\text{A.3b})$$

denote the eigenvalues of  $e^{\beta \mu/2} T_1$ . In the thermodynamic limit  $M \rightarrow \infty$ ,  $N/M = \rho$  (density), we have  $Z_1^{(2)} = \lambda_1^M$  because  $\lambda_1 > |\lambda_2|$  and  $\lambda_1 > |\sinh(t + \mu/2)\beta|$ . To determine  $\mu = \mu(\beta, \rho)$  we use

$$\rho \equiv \frac{1}{M} \sum_{i=1}^M \langle n_i \rangle = \frac{1}{M} \frac{\partial}{\partial \beta \mu} \ln Z_1^{(2)} = \frac{1}{\lambda_1} \frac{\partial}{\partial \beta \mu} \lambda_1 \\ = \frac{1}{2\lambda_1} \left\{ e^{\beta(\mu - v)} - \left[ (1 - e^{\beta(\mu - v)}) e^{\beta(\mu - v)} - 2e^{\beta \mu} \cosh^2 \beta t \right] X \right. \\ \left. \times \left[ (1 - e^{\beta(\mu - v)})^2 + 4e^{\beta \mu} \cosh^2 \beta t \right]^{-1/2} \right\} \quad (\text{A.4})$$

In general, this equation has to be solved numerically. In the case of  $\rho = 1/2$ , a half-filled band, one can solve Eq. (A.4) by putting  $\mu = v$ . In this case the partition function reads

$$Z_1^{(2)} = \{1 + e^{\beta v/2} \cosh(\beta t)\}^M \quad (\text{A.5})$$

In the special case  $v = 2t$  the energy and specific heat per site are given by

$$E_1^{(2)} / M = -t(e^{2\beta t} - 3)(e^{2\beta t} + 3)^{-1} \quad (\text{A.6a})$$

and

$$C_1^{(2)} / M = 3(2\beta t)^2 e^{2\beta t} (e^{2\beta t} + 3)^{-2} \quad (\text{A.6b})$$

For comparison, the numerical values for the energy and specific heat per site for this particular choice of  $t$ ,  $v$ , and  $\rho$  have also been included in Tables III and IV.

Finally, we would like to mention that one can also obtain analytic expressions for the density-density correlation functions in the special case  $m = 1$ , and one finds that they decay exponentially with distance.

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